A simplex-type Voronoi algorithm based on short vector computations of copositive quadratic forms

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based on work with Mathieu Dutour Sikirić and Frank Vallentin
Perfect Forms \hspace{1cm} (for $Q \in S_{>0}^n$ positive definite)

- $\min(Q) = \min_{x \in \mathbb{Z}^n \setminus \{0\}} Q[x]$ is the \textbf{arithmetical minimum} of $Q$

  $Q$ is uniquely determined by $\min(Q)$ and

- $Q$ \textbf{perfect} $\iff$ $\text{Min}Q = \{ x \in \mathbb{Z}^n : Q[x] = \min(Q) \}$

- $V(Q) = \text{cone}\{xx^t : x \in \text{Min}Q\}$ is \textbf{Voronoi cone} of $Q$

  (Voronoi cones are full dimensional if and only if $Q$ is perfect!)

\textbf{THM:} Voronoi cones give a polyhedral tessellation of $S_{>0}^n$ and there are only finitely many up to $\text{GL}_n(\mathbb{Z})$-equivalence.
Voronoi’s Reduction Theory

\[ \text{GL}_n(\mathbb{Z}) \text{ acts on } S^n_{>0} \text{ by } Q \mapsto U^tQU \]

Task of a reduction theory is to provide a fundamental domain

Voronoi’s algorithm gives a recipe for the construction of a complete list of such polyhedral cones up to \( \text{GL}_n(\mathbb{Z}) \)-equivalence
Ryshkov Polyhedron

The set of all positive definite quadratic forms / matrices with arithmetical minimum at least 1 is called Ryshkov polyhedron

\[ \mathcal{R} = \left\{ Q \in S^n_{>0} : Q[x] \geq 1 \text{ for all } x \in \mathbb{Z}^n \setminus \{0\} \right\} \]

- \( \mathcal{R} \) is a locally finite polyhedron
- Vertices of \( \mathcal{R} \) are perfect
Voronoi’s Algorithm

Start with a perfect form $Q$

1. **SVP**: Compute $\text{Min } Q$ and describing inequalities of the polyhedral cone
   $$\mathcal{P}(Q) = \{ Q' \in S^n : Q'[x] \geq 1 \text{ for all } x \in \text{Min } Q \}$$

2. **PolyRepConv**: Enumerate extreme rays $R_1, \ldots, R_k$ of $\mathcal{P}(Q)$

3. **SVPs**: Determine contiguous perfect forms $Q_i = Q + \alpha R_i$, $i = 1, \ldots, k$

4. **ISOMs**: Test if $Q_i$ is arithmetically equivalent to a known form

5. Repeat steps 1.–4. for new perfect forms

( graph traversal search on edge graph of Ryshkov polyhedron )
Generalization

IDEA: Generalize Voronoi’s theory to other convex cones and their duals
(Opgenorth, 2001)

In particular to the completely positive cone

\[ \mathcal{CP}_n = \text{cone}\{xx^T : x \in \mathbb{R}_{\geq 0}^n\} \quad \text{and its dual, the copositive cone} \]

\[ \mathcal{COP}_n = (\mathcal{CP}_n)^* = \{ B \in S^n : \langle A, B \rangle \geq 0 \text{ for all } A \in \mathcal{CP}_n \} \]

\[ = \{ B \in S^n : B[x] \geq 0 \text{ for all } x \in \mathbb{R}_{\geq 0}^n \} \]

\[ \mathcal{CP}_n \subset S_{\geq 0}^n \subset \mathcal{COP}_n \]

\[ \langle A, B \rangle = \text{Trace}(A \cdot B) \] denotes the standard inner product on \( S^n \)
Application: Copositive Optimization

- Copositive optimization problems are **convex conic problems**

\[
\min \langle C, Q \rangle \text{ such that } \langle Q, A_i \rangle = b_i, \ i = 1, \ldots, m
\]

and \( Q \in \text{CONE} \)

\[
\text{CONE} = \mathbb{R}^n_{\geq 0}
\]

**Linear Programming (LP)**

\[
\text{CONE} = S^n_{\geq 0}
\]

**Semidefinite Programming (SDP)**

\[
\text{CONE} = \mathcal{CP}_n \text{ or } \mathcal{COP}_n
\]

**Copositive Programming (CP)**

**Task:** Certify or disprove \( Q \in \tilde{\mathcal{P}}_n = \text{cone} \{ xx^\top : x \in \mathbb{Q}^n_{\geq 0} \} \)

( due to duality theory we can give certificates for solutions of convex conic problems )
Copositive minimum

**DEF:** \( \min_{COP} Q = \min_{x \in \mathbb{Z}_+^n \setminus \{0\}} Q[x] \) is the copositive minimum

Difficult to compute!?

**THM:** (Bundfuss and Dür, 2008)

For \( Q \in \text{int} COP_n \) we can construct a family of simplices \( \Delta^k \) in the standard simplex \( \Delta = \{ x \in \mathbb{R}_+^n : x_1 + \ldots + x_n = 1 \} \) such that each \( \Delta^k \) has vertices \( v_1, \ldots, v_n \) with \( v_i^T Q v_j > 0 \)

A first naive algorithm:

"Fincke-Pohst strategy" to compute \( \min_{COP} Q \) in each cone \( \Delta^k \)
Generalized Ryshkov polyhedron

The set of all copositive quadratic forms / matrices with copositive minimum at least 1 is called Ryshkov polyhedron

\[ \mathcal{R} = \{ Q \in \text{COP}_n : Q[x] \geq 1 \text{ for all } x \in \mathbb{Z}_{\geq 0}^n \setminus \{0\} \} \]

**DEF:** \( Q \in \text{int COP}_n \) is called **COP-perfect** if and only if

\[ Q \text{ is uniquely determined by } \min_{\text{COP}} Q \text{ and} \]

\[ \text{Min}_{\text{COP}} Q = \{ x \in \mathbb{Z}_{\geq 0}^n : Q[x] = \min_{\text{COP}} Q \} \]

- \( \mathcal{R} \) is a **locally finite polyhedron** (with dead-ends / rays)
- Vertices of \( \mathcal{R} \) are **COP**-perfect
A copositive starting point

\[
\begin{pmatrix}
2 & -1 & 0 & \ldots & 0 \\
-1 & 2 & \ddots & \ddots & \vdots \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & 2 & -1 \\
0 & \ldots & 0 & -1 & 2
\end{pmatrix}
\]

is \(\text{COP}\)-perfect

**Proof.** Matrix \(Q_{A_n}\) is positive definite since

\[
Q_{A_n}[x] = x_1^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2 + x_n^2 \quad \text{for } x \in \mathbb{R}.
\]

In particular it lies in the interior of the copositive cone. Furthermore,

\[
\min_{\text{COP}} Q_{A_n} = 2 \quad \text{with} \quad \text{Min}_{\text{COP}} Q_{A_n} = \left\{ \sum_{i=j}^{k} e_j : 1 \leq j \leq k \leq n \right\}
\]
Voronoi-type simplex algorithm

Input: $A \in S^n$

Obtain an initial $\text{COP}$-perfect matrix $B_P$

1. if $\langle B_P, A \rangle < 0$ then output $A \not\in CP_n$ (with witness $B_P$)
2. LP: if $A \in \text{cone} \{ xx^\top : x \in \text{Min}_{\text{COP}} B_P \}$ then output $A \in \tilde{CP}_n$
3. COP-SVP: Compute $\text{Min}_{\text{COP}} B_P$ and the polyhedral cone
   
   $$\mathcal{P}(B_P) = \{ B \in S^n : B[x] \geq 1 \text{ for all } x \in \text{Min}_{\text{COP}} B_P \}$$

4. PolyRepConv: Determine a generator $R$ of an extreme ray of $\mathcal{P}(B_P)$
   with $\langle A, R \rangle < 0$. \hspace{1cm} (flexible ”pivot-rule”)

5. SimplexDiv: if $R \in \text{COP}_n$ then output $A \not\in CP_n$ (with witness $R$)

6. COP-SVPs: Determine the contiguous $\text{COP}$-perfect matrix
   $$B_N := B_P + \lambda R \text{ with } \lambda > 0 \text{ and } \text{min}_{\text{COP}} B_N = 1$$

7. Set $B_P := B_N$ and goto 1.
Interior cases
(algorithm terminates)

EX: \[ A = \begin{pmatrix} 6 & 3 \\ 3 & 2 \end{pmatrix} \]

Starting with \( Q_{A_2} \) one iteration of the algorithm finds the \( COP \)-perfect matrix \( B_P = \begin{pmatrix} 1 & -3/2 \\ -3/2 & 3 \end{pmatrix} \)

\[ A = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}^\top + \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}^\top + \begin{pmatrix} 2 \\ 1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix}^\top \]
Boundary cases from $\mathcal{CP}_n$
(algorithm terminates with a suitable pivot-rule)

EX: \[
\begin{pmatrix}
8 & 5 & 1 & 1 & 5 \\
5 & 8 & 5 & 1 & 1 \\
1 & 5 & 8 & 5 & 1 \\
1 & 1 & 5 & 8 & 5 \\
5 & 1 & 1 & 5 & 8 \\
\end{pmatrix}
\]

from Groetzner, Dür (2018)

Starting with $Q_{A_5}$, our algorithm finds a cp-factorization after 5 iterations

\begin{align*}
v_1 &= (0, 0, 0, 1, 1) & v_6 &= (1, 0, 0, 0, 1) \\
v_2 &= (0, 0, 1, 1, 0) & v_7 &= (1, 0, 0, 1, 2) \\
v_3 &= (0, 0, 1, 2, 1) & v_8 &= (1, 1, 0, 0, 0) \\
v_4 &= (0, 1, 1, 0, 0) & v_9 &= (1, 2, 1, 0, 0) \\
v_5 &= (0, 1, 2, 1, 0) & v_{10} &= (2, 1, 0, 0, 1)
\end{align*}

giving a certificate for the matrix to be completely positive
Exterior cases
(algorithm conjectured to terminate)

\[
\begin{pmatrix}
1 & 1 & 0 & 0 & 1 \\
1 & 2 & 1 & 0 & 0 \\
0 & 1 & 2 & 1 & 0 \\
0 & 0 & 1 & 2 & 1 \\
1 & 0 & 0 & 1 & 6
\end{pmatrix}
\]

EX: from Nie (2014)

Starting with \( Q_{A_5} \), after 18 iterations our algorithm finds the \( \text{COP} \)-perfect

\[
\begin{pmatrix}
363/5 & -2126/35 & 2879/70 & 608/21 & -4519/210 \\
-2126/35 & 1787/35 & -347/10 & 1025/42 & 253/14 \\
2879/70 & -347/10 & 829/35 & -1748/105 & 371/30 \\
608/21 & 1025/42 & -1748/105 & 1237/105 & -601/70 \\
-4519/210 & 253/14 & 371/30 & -601/70 & 671/105
\end{pmatrix}
\]

giving a certificate for the matrix not to be completely positive
Open Questions / TODOs

• Find suitable / good pivot rules for boundary cases

• Prove termination of algorithm for exterior cases

• Improve computations in practice

• … in particular: find a better algorithm to compute $\min_{\text{COP}}$ and the set of its representatives $\text{Min}_{\text{COP}}$ (COP-SVPs)
References

• Achill Schürmann, *Computational Geometry of Positive Definite Quadratic Forms*, University Lecture Series, AMS, Providence, RI, 2009.


• Mathieu Dutour Sikirić, Achill Schürmann and Frank Vallentin, A simplex algorithm for rational cp-factorization, Math. Prog. A, 2020, online first

THANKS!